

Numerical Recipes in Fortran 77

The Art of Scientific Computing
Second Edition

Volume 1 of
Fortran Numerical Recipes

William H. Press

Harvard-Smithsonian Center for Astrophysics

Saul A. Teukolsky

Department of Physics, Cornell University

William T. Vetterling

Polaroid Corporation

Brian P. Flannery

EXXON Research and Engineering Company

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one), to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website <http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

Published by the Press Syndicate of the University of Cambridge
The Pitt Building, Trumpington Street, Cambridge CB2 1RP
40 West 20th Street, New York, NY 10011-4211, USA
10 Stamford Road, Oakleigh, Melbourne 3166, Australia

Copyright © Cambridge University Press 1986, 1992
except for §13.10, which is placed into the public domain,
and except for all other computer programs and procedures, which are
Copyright © Numerical Recipes Software 1986, 1992, 1997
All Rights Reserved.

Some sections of this book were originally published, in different form, in *Computers in Physics* magazine, Copyright © American Institute of Physics, 1988–1992.

First Edition originally published 1986; Second Edition originally published 1992 as *Numerical Recipes in FORTRAN: The Art of Scientific Computing*
Reprinted with corrections, 1993, 1994, 1995.
Reprinted with corrections, 1996, 1997, 2001, as *Numerical Recipes in Fortran 77: The Art of Scientific Computing* (Vol. 1 of Fortran Numerical Recipes)

This reprinting is corrected to software version 2.10

Printed in the United States of America
Typeset in \TeX

Without an additional license to use the contained software, this book is intended as a text and reference book, for reading purposes only. A free license for limited use of the software by the individual owner of a copy of this book who personally types one or more routines into a single computer is granted under terms described on p. xxi. See the section “License Information” (pp. xx–xxiii) for information on obtaining more general licenses at low cost.

Machine-readable media containing the software in this book, with included licenses for use on a single screen, are available from Cambridge University Press. See the order form at the back of the book, email to “orders@cup.org” (North America) or “trade@cup.cam.ac.uk” (rest of world), or write to Cambridge University Press, 110 Midland Avenue, Port Chester, NY 10573 (USA), for further information.

The software may also be downloaded, with immediate purchase of a license also possible, from the Numerical Recipes Software Web Site (<http://www.nr.com>). Unlicensed transfer of Numerical Recipes programs to any other format, or to any computer except one that is specifically licensed, is strictly prohibited. Technical questions, corrections, and requests for information should be addressed to Numerical Recipes Software, P.O. Box 243, Cambridge, MA 02238 (USA), email “info@nr.com”, or fax 781 863-1739.

Library of Congress Cataloging in Publication Data

Numerical recipes in Fortran 77 : the art of scientific computing / William H. Press
... [et al.]. — 2nd ed.

Includes bibliographical references (p.) and index.

ISBN 0-521-43064-X

1. Numerical analysis—Computer programs. 2. Science—Mathematics—Computer programs.
3. FORTRAN (Computer program language) I. Press, William H.

QA297.N866 1992

519.4'0285'53—dc20

92-8876

A catalog record for this book is available from the British Library.

ISBN 0 521 43064 X Volume 1 (this book)
ISBN 0 521 57439 0 Volume 2
ISBN 0 521 43721 0 Example book in FORTRAN
ISBN 0 521 57440 4 FORTRAN diskette (IBM 3.5'')
ISBN 0 521 57608 3 CDROM (IBM PC/Macintosh)
ISBN 0 521 57607 5 CDROM (UNIX)

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one), to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website <http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

Contents

<i>Plan of the Two-Volume Edition</i>	<i>xiii</i>
<i>Preface to the Second Edition</i>	<i>xv</i>
<i>Preface to the First Edition</i>	<i>xviii</i>
<i>License Information</i>	<i>xx</i>
<i>Computer Programs by Chapter and Section</i>	<i>xxiv</i>
1 Preliminaries	1
1.0 Introduction	1
1.1 Program Organization and Control Structures	5
1.2 Error, Accuracy, and Stability	18
2 Solution of Linear Algebraic Equations	22
2.0 Introduction	22
2.1 Gauss-Jordan Elimination	27
2.2 Gaussian Elimination with Backsubstitution	33
2.3 LU Decomposition and Its Applications	34
2.4 Tridiagonal and Band Diagonal Systems of Equations	42
2.5 Iterative Improvement of a Solution to Linear Equations	47
2.6 Singular Value Decomposition	51
2.7 Sparse Linear Systems	63
2.8 Vandermonde Matrices and Toeplitz Matrices	82
2.9 Cholesky Decomposition	89
2.10 QR Decomposition	91
2.11 Is Matrix Inversion an N^3 Process?	95
3 Interpolation and Extrapolation	99
3.0 Introduction	99
3.1 Polynomial Interpolation and Extrapolation	102
3.2 Rational Function Interpolation and Extrapolation	104
3.3 Cubic Spline Interpolation	107
3.4 How to Search an Ordered Table	110
3.5 Coefficients of the Interpolating Polynomial	113
3.6 Interpolation in Two or More Dimensions	116

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
 Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
 Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one), to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website <http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

4	<i>Integration of Functions</i>	123
4.0	Introduction	123
4.1	Classical Formulas for Equally Spaced Abscissas	124
4.2	Elementary Algorithms	130
4.3	Romberg Integration	134
4.4	Improper Integrals	135
4.5	Gaussian Quadratures and Orthogonal Polynomials	140
4.6	Multidimensional Integrals	155
5	<i>Evaluation of Functions</i>	159
5.0	Introduction	159
5.1	Series and Their Convergence	159
5.2	Evaluation of Continued Fractions	163
5.3	Polynomials and Rational Functions	167
5.4	Complex Arithmetic	171
5.5	Recurrence Relations and Clenshaw's Recurrence Formula	172
5.6	Quadratic and Cubic Equations	178
5.7	Numerical Derivatives	180
5.8	Chebyshev Approximation	184
5.9	Derivatives or Integrals of a Chebyshev-approximated Function	189
5.10	Polynomial Approximation from Chebyshev Coefficients	191
5.11	Economization of Power Series	192
5.12	Padé Approximants	194
5.13	Rational Chebyshev Approximation	197
5.14	Evaluation of Functions by Path Integration	201
6	<i>Special Functions</i>	205
6.0	Introduction	205
6.1	Gamma Function, Beta Function, Factorials, Binomial Coefficients	206
6.2	Incomplete Gamma Function, Error Function, Chi-Square Probability Function, Cumulative Poisson Function	209
6.3	Exponential Integrals	215
6.4	Incomplete Beta Function, Student's Distribution, F-Distribution, Cumulative Binomial Distribution	219
6.5	Bessel Functions of Integer Order	223
6.6	Modified Bessel Functions of Integer Order	229
6.7	Bessel Functions of Fractional Order, Airy Functions, Spherical Bessel Functions	234
6.8	Spherical Harmonics	246
6.9	Fresnel Integrals, Cosine and Sine Integrals	248
6.10	Dawson's Integral	252
6.11	Elliptic Integrals and Jacobian Elliptic Functions	254
6.12	Hypergeometric Functions	263
7	<i>Random Numbers</i>	266
7.0	Introduction	266
7.1	Uniform Deviates	267

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
 Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
 Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-
 readable files (including this one), to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website
<http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

7.2 Transformation Method: Exponential and Normal Deviates	277
7.3 Rejection Method: Gamma, Poisson, Binomial Deviates	281
7.4 Generation of Random Bits	287
7.5 Random Sequences Based on Data Encryption	290
7.6 Simple Monte Carlo Integration	295
7.7 Quasi- (that is, Sub-) Random Sequences	299
7.8 Adaptive and Recursive Monte Carlo Methods	306
8 Sorting	320
8.0 Introduction	320
8.1 Straight Insertion and Shell's Method	321
8.2 Quicksort	323
8.3 Heapsort	327
8.4 Indexing and Ranking	329
8.5 Selecting the M th Largest	333
8.6 Determination of Equivalence Classes	337
9 Root Finding and Nonlinear Sets of Equations	340
9.0 Introduction	340
9.1 Bracketing and Bisection	343
9.2 Secant Method, False Position Method, and Ridder's Method	347
9.3 Van Wijngaarden–Dekker–Brent Method	352
9.4 Newton–Raphson Method Using Derivative	355
9.5 Roots of Polynomials	362
9.6 Newton–Raphson Method for Nonlinear Systems of Equations	372
9.7 Globally Convergent Methods for Nonlinear Systems of Equations	376
10 Minimization or Maximization of Functions	387
10.0 Introduction	387
10.1 Golden Section Search in One Dimension	390
10.2 Parabolic Interpolation and Brent's Method in One Dimension	395
10.3 One-Dimensional Search with First Derivatives	399
10.4 Downhill Simplex Method in Multidimensions	402
10.5 Direction Set (Powell's) Methods in Multidimensions	406
10.6 Conjugate Gradient Methods in Multidimensions	413
10.7 Variable Metric Methods in Multidimensions	418
10.8 Linear Programming and the Simplex Method	423
10.9 Simulated Annealing Methods	436
11 Eigensystems	449
11.0 Introduction	449
11.1 Jacobi Transformations of a Symmetric Matrix	456
11.2 Reduction of a Symmetric Matrix to Tridiagonal Form: Givens and Householder Reductions	462
11.3 Eigenvalues and Eigenvectors of a Tridiagonal Matrix	469
11.4 Hermitian Matrices	475
11.5 Reduction of a General Matrix to Hessenberg Form	476

11.6 The QR Algorithm for Real Hessenberg Matrices	480
11.7 Improving Eigenvalues and/or Finding Eigenvectors by Inverse Iteration	487
12 Fast Fourier Transform	490
12.0 Introduction	490
12.1 Fourier Transform of Discretely Sampled Data	494
12.2 Fast Fourier Transform (FFT)	498
12.3 FFT of Real Functions, Sine and Cosine Transforms	504
12.4 FFT in Two or More Dimensions	515
12.5 Fourier Transforms of Real Data in Two and Three Dimensions	519
12.6 External Storage or Memory-Local FFTs	525
13 Fourier and Spectral Applications	530
13.0 Introduction	530
13.1 Convolution and Deconvolution Using the FFT	531
13.2 Correlation and Autocorrelation Using the FFT	538
13.3 Optimal (Wiener) Filtering with the FFT	539
13.4 Power Spectrum Estimation Using the FFT	542
13.5 Digital Filtering in the Time Domain	551
13.6 Linear Prediction and Linear Predictive Coding	557
13.7 Power Spectrum Estimation by the Maximum Entropy (All Poles) Method	565
13.8 Spectral Analysis of Unevenly Sampled Data	569
13.9 Computing Fourier Integrals Using the FFT	577
13.10 Wavelet Transforms	584
13.11 Numerical Use of the Sampling Theorem	600
14 Statistical Description of Data	603
14.0 Introduction	603
14.1 Moments of a Distribution: Mean, Variance, Skewness, and So Forth	604
14.2 Do Two Distributions Have the Same Means or Variances?	609
14.3 Are Two Distributions Different?	614
14.4 Contingency Table Analysis of Two Distributions	622
14.5 Linear Correlation	630
14.6 Nonparametric or Rank Correlation	633
14.7 Do Two-Dimensional Distributions Differ?	640
14.8 Savitzky-Golay Smoothing Filters	644
15 Modeling of Data	650
15.0 Introduction	650
15.1 Least Squares as a Maximum Likelihood Estimator	651
15.2 Fitting Data to a Straight Line	655
15.3 Straight-Line Data with Errors in Both Coordinates	660
15.4 General Linear Least Squares	665
15.5 Nonlinear Models	675

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
 Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
 Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one), to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website <http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

15.6 Confidence Limits on Estimated Model Parameters	684
15.7 Robust Estimation	694
16 Integration of Ordinary Differential Equations	701
16.0 Introduction	701
16.1 Runge-Kutta Method	704
16.2 Adaptive Stepsize Control for Runge-Kutta	708
16.3 Modified Midpoint Method	716
16.4 Richardson Extrapolation and the Bulirsch-Stoer Method	718
16.5 Second-Order Conservative Equations	726
16.6 Stiff Sets of Equations	727
16.7 Multistep, Multivalued, and Predictor-Corrector Methods	740
17 Two Point Boundary Value Problems	745
17.0 Introduction	745
17.1 The Shooting Method	749
17.2 Shooting to a Fitting Point	751
17.3 Relaxation Methods	753
17.4 A Worked Example: Spheroidal Harmonics	764
17.5 Automated Allocation of Mesh Points	774
17.6 Handling Internal Boundary Conditions or Singular Points	775
18 Integral Equations and Inverse Theory	779
18.0 Introduction	779
18.1 Fredholm Equations of the Second Kind	782
18.2 Volterra Equations	786
18.3 Integral Equations with Singular Kernels	788
18.4 Inverse Problems and the Use of A Priori Information	795
18.5 Linear Regularization Methods	799
18.6 Backus-Gilbert Method	806
18.7 Maximum Entropy Image Restoration	809
19 Partial Differential Equations	818
19.0 Introduction	818
19.1 Flux-Conservative Initial Value Problems	825
19.2 Diffusive Initial Value Problems	838
19.3 Initial Value Problems in Multidimensions	844
19.4 Fourier and Cyclic Reduction Methods for Boundary Value Problems	848
19.5 Relaxation Methods for Boundary Value Problems	854
19.6 Multigrid Methods for Boundary Value Problems	862
20 Less-Numerical Algorithms	881
20.0 Introduction	881
20.1 Diagnosing Machine Parameters	881
20.2 Gray Codes	886

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
 Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
 Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one), to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website <http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

20.3 Cyclic Redundancy and Other Checksums	888
20.4 Huffman Coding and Compression of Data	896
20.5 Arithmetic Coding	902
20.6 Arithmetic at Arbitrary Precision	906
References for Volume 1	916
Index of Programs and Dependencies (Vol. 1)	921
General Index to Volumes 1 and 2	
 Contents of Volume 2: Numerical Recipes in Fortran 90	
Preface to Volume 2	viii
Foreword by Michael Metcalf	x
License Information	xvii
21 Introduction to Fortran 90 Language Features	935
22 Introduction to Parallel Programming	962
23 Numerical Recipes Utilities for Fortran 90	987
Fortran 90 Code Chapters	1009
B1 Preliminaries	1010
B2 Solution of Linear Algebraic Equations	1014
B3 Interpolation and Extrapolation	1043
B4 Integration of Functions	1052
B5 Evaluation of Functions	1070
B6 Special Functions	1083
B7 Random Numbers	1141
B8 Sorting	1167
B9 Root Finding and Nonlinear Sets of Equations	1182
B10 Minimization or Maximization of Functions	1201
B11 Eigensystems	1225
B12 Fast Fourier Transform	1235

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
 Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
 Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one), to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website <http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

B13	<i>Fourier and Spectral Applications</i>	1253
B14	<i>Statistical Description of Data</i>	1269
B15	<i>Modeling of Data</i>	1285
B16	<i>Integration of Ordinary Differential Equations</i>	1297
B17	<i>Two Point Boundary Value Problems</i>	1314
B18	<i>Integral Equations and Inverse Theory</i>	1325
B19	<i>Partial Differential Equations</i>	1332
B20	<i>Less-Numerical Algorithms</i>	1343
	<i>References for Volume 2</i>	1359
	<i>Appendices</i>	
C1	<i>Listing of Utility Modules (nrtype and nrutil)</i>	1361
C2	<i>Listing of Explicit Interfaces</i>	1384
C3	<i>Index of Programs and Dependencies (Vol. 2)</i>	1434
	<i>General Index to Volumes 1 and 2</i>	1447

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one), to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website <http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-
readable files (including this one), to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website
<http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

Plan of the Two-Volume Edition

Fortran, long the epitome of stability, is once again a language in flux. Fortran 90 is not just the long-awaited updating of traditional Fortran 77 to modern computing practices, but also demonstrates Fortran's decisive bid to be the language of choice for parallel programming on multiprocessor computers.

At the same time, Fortran 90 is completely backwards-compatible with all Fortran 77 code. So, users with legacy code, or who choose to use only older language constructs, will still get the benefit of updated and actively maintained compilers.

As we, the authors of *Numerical Recipes*, watched the gestation and birth of Fortran 90 by its governing standards committee (an interesting process described by a leading Committee member, Michael Metcalf, in the Foreword to our Volume 2), it became clear to us that the right moment for moving *Numerical Recipes* from Fortran 77 to Fortran 90 was sooner, rather than later.

On the other hand, it was equally clear that Fortran-77-style programming — no matter whether with Fortran 77 or Fortran 90 compilers — is, and will continue for a long time to be, the “mother tongue” of a large population of active scientists, engineers, and other users of numerical computation. This is not a user base that we would willingly or knowingly abandon.

The solution was immediately clear: a two-volume edition of the Fortran *Numerical Recipes* consisting of Volume 1 (this one, a corrected reprinting of the previous one-volume edition), now retitled *Numerical Recipes in Fortran 77*, and a completely new Volume 2, titled *Numerical Recipes in Fortran 90: The Art of Parallel Scientific Computing*. Volume 2 begins with three chapters (21, 22, and 23) that extend the narrative of the first volume to the new subjects of Fortran 90 language features, parallel programming methodology, and the implementation of certain useful utility functions in Fortran 90. Then, in exact correspondence with Volume 1's Chapters 1–20, are new chapters B1–B20, devoted principally to the listing and explanation of new Fortran 90 routines. With a few exceptions, each Fortran 77 routine in Volume 1 has a corresponding new Fortran 90 version in Volume 2. (The exceptions are a few new capabilities, notably in random number generation and in multigrid PDE solvers, that are unique to Volume 2's Fortran 90.) Otherwise, there is no duplication between the volumes. The detailed explanation of the algorithms in this Volume 1 is intended to apply to, and be essential for, both volumes.

In other words: **You can use this Volume 1 without having Volume 2, but you can't use Volume 2 without Volume 1.** We think that there is much to be gained by having and using *both* volumes: Fortran 90's parallel language constructions are not only useful for present and future multiprocessor machines; they also allow for the elegant and concise formulation of many algorithms on ordinary single-processor computers. We think that essentially *all* Fortran programmers will want gradually to migrate into Fortran 90 and into a mode of “thinking parallel.” We have written Volume 2 specifically to help with this important transition.

Volume 2's discussion of parallel programming is focused on those issues of direct relevance to the Fortran 90 programmer. Some more general aspects of parallel programming, such as communication costs, synchronization of multiple processors, etc., are touched on only briefly. We provide references to the extensive literature on these more specialized topics.

A special note to C programmers: Right now, there is no effort at producing a parallel version of C that is comparable to Fortran 90 in maturity, acceptance, and stability. We think, therefore, that C programmers will be well served by using Volume 2, either in conjunction with this Volume 1 or else in conjunction with the sister volume *Numerical Recipes in C: The Art of Scientific Computing*, for an educational excursion into Fortran 90, its parallel programming constructions, and the numerical algorithms that capitalize on them. C and C++ programming have not been far from our minds as we have written this two-volume version. We think you will find that time spent in absorbing the principal lessons of Volume 2's Chapters 21–23 will be amply repaid in the future, as C and C++ eventually develop standard parallel extensions.

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one) to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website <http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

Preface to the Second Edition

Our aim in writing the original edition of *Numerical Recipes* was to provide a book that combined general discussion, analytical mathematics, algorithmics, and actual working programs. The success of the first edition puts us now in a difficult, though hardly unenviable, position. We wanted, then and now, to write a book that is informal, fearlessly editorial, unesoteric, and above all useful. There is a danger that, if we are not careful, we might produce a second edition that is weighty, balanced, scholarly, and boring.

It is a mixed blessing that we know more now than we did six years ago. Then, we were making educated guesses, based on existing literature and our own research, about which numerical techniques were the most important and robust. Now, we have the benefit of direct feedback from a large reader community. Letters to our alter-ego enterprise, Numerical Recipes Software, are in the thousands per year. (Please, *don't telephone* us.) Our post office box has become a magnet for letters pointing out that we have omitted some particular technique, well known to be important in a particular field of science or engineering. We value such letters, and digest them carefully, especially when they point us to specific references in the literature.

The inevitable result of this input is that this Second Edition of *Numerical Recipes* is substantially larger than its predecessor, in fact about 50% larger both in words and number of included programs (the latter now numbering well over 300). “Don’t let the book grow in size,” is the advice that we received from several wise colleagues. We have tried to follow the intended spirit of that advice, even as we violate the letter of it. We have not lengthened, or increased in difficulty, the book’s principal discussions of mainstream topics. Many new topics are presented at this same accessible level. Some topics, both from the earlier edition and new to this one, are now set in smaller type that labels them as being “advanced.” The reader who ignores such advanced sections completely will not, we think, find any lack of continuity in the shorter volume that results.

Here are some highlights of the new material in this Second Edition:

- a new chapter on integral equations and inverse methods
- a detailed treatment of multigrid methods for solving elliptic partial differential equations
- routines for band diagonal linear systems
- improved routines for linear algebra on sparse matrices
- Cholesky and QR decomposition
- orthogonal polynomials and Gaussian quadratures for arbitrary weight functions
- methods for calculating numerical derivatives
- Padé approximants, and rational Chebyshev approximation
- Bessel functions, and modified Bessel functions, of fractional order; and several other new special functions
- improved random number routines
- quasi-random sequences
- routines for adaptive and recursive Monte Carlo integration in high-dimensional spaces
- globally convergent methods for sets of nonlinear equations

- simulated annealing minimization for continuous control spaces
- fast Fourier transform (FFT) for real data in two and three dimensions
- fast Fourier transform (FFT) using external storage
- improved fast cosine transform routines
- wavelet transforms
- Fourier integrals with upper and lower limits
- spectral analysis on unevenly sampled data
- Savitzky-Golay smoothing filters
- fitting straight line data with errors in both coordinates
- a two-dimensional Kolmogorov-Smirnoff test
- the statistical bootstrap method
- embedded Runge-Kutta-Fehlberg methods for differential equations
- high-order methods for stiff differential equations
- a new chapter on “less-numerical” algorithms, including Huffman and arithmetic coding, arbitrary precision arithmetic, and several other topics.

Consult the Preface to the First Edition, following, or the Table of Contents, for a list of the more “basic” subjects treated.

Acknowledgments

It is not possible for us to list by name here all the readers who have made useful suggestions; we are grateful for these. In the text, we attempt to give specific attribution for ideas that appear to be original, and not known in the literature. We apologize in advance for any omissions.

Some readers and colleagues have been particularly generous in providing us with ideas, comments, suggestions, and programs for this Second Edition. We especially want to thank George Rybicki, Philip Pinto, Peter Lepage, Robert Lupton, Douglas Eardley, Ramesh Narayan, David Spergel, Alan Oppenheim, Sallie Baliunas, Scott Tremaine, Glennys Farrar, Steven Block, John Peacock, Thomas Loredo, Matthew Choptuik, Gregory Cook, L. Samuel Finn, P. Deuflhard, Harold Lewis, Peter Weinberger, David Syer, Richard Ferch, Steven Epstein, and William Gould. We have been helped by Nancy Lee Snyder’s mastery of a complicated \TeX manuscript. We express appreciation to our editors Lauren Cowles and Alan Harvey at Cambridge University Press, and to our production editor Russell Hahn. We remain, of course, grateful to the individuals acknowledged in the Preface to the First Edition.

Special acknowledgment is due to programming consultant Seth Finkelstein, who influenced many of the routines in this book, and wrote or rewrote many more routines in its C-language twin and the companion Example books. Our project has benefited enormously from Seth’s talent for detecting, and following the trail of, even very slight anomalies (often compiler bugs, but occasionally our errors), and from his good programming sense.

We prepared this book for publication on DEC and Sun workstations running the UNIX operating system, and on a 486/33 PC compatible running MS-DOS 5.0/Windows 3.0. (See §1.0 for a list of additional computers used in program tests.) We enthusiastically recommend the principal software used: GNU Emacs, \TeX , Perl, Adobe Illustrator, and PostScript. Also used were a variety of FORTRAN compilers — too numerous (and sometimes too buggy) for individual

acknowledgment. It is a sobering fact that our standard test suite (exercising all the routines in this book) has uncovered compiler bugs in a large majority of the compilers tried. When possible, we work with developers to see that such bugs get fixed; we encourage interested compiler developers to contact us about such arrangements.

WHP and SAT acknowledge the continued support of the U.S. National Science Foundation for their research on computational methods. D.A.R.P.A. support is acknowledged for §13.10 on wavelets.

June, 1992

William H. Press
Saul A. Teukolsky
William T. Vetterling
Brian P. Flannery

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one) to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website <http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

Preface to the First Edition

We call this book *Numerical Recipes* for several reasons. In one sense, this book is indeed a “cookbook” on numerical computation. However there is an important distinction between a cookbook and a restaurant menu. The latter presents choices among complete dishes in each of which the individual flavors are blended and disguised. The former — and this book — reveals the individual ingredients and explains how they are prepared and combined.

Another purpose of the title is to connote an eclectic mixture of presentational techniques. This book is unique, we think, in offering, for each topic considered, a certain amount of general discussion, a certain amount of analytical mathematics, a certain amount of discussion of algorithmics, and (most important) actual implementations of these ideas in the form of working computer routines. Our task has been to find the right balance among these ingredients for each topic. You will find that for some topics we have tilted quite far to the analytic side; this where we have felt there to be gaps in the “standard” mathematical training. For other topics, where the mathematical prerequisites are universally held, we have tilted towards more in-depth discussion of the nature of the computational algorithms, or towards practical questions of implementation.

We admit, therefore, to some unevenness in the “level” of this book. About half of it is suitable for an advanced undergraduate course on numerical computation for science or engineering majors. The other half ranges from the level of a graduate course to that of a professional reference. Most cookbooks have, after all, recipes at varying levels of complexity. An attractive feature of this approach, we think, is that the reader can use the book at increasing levels of sophistication as his/her experience grows. Even inexperienced readers should be able to use our most advanced routines as black boxes. Having done so, we hope that these readers will subsequently go back and learn what secrets are inside.

If there is a single dominant theme in this book, it is that practical methods of numerical computation can be simultaneously efficient, clever, and — important — clear. The alternative viewpoint, that efficient computational methods must necessarily be so arcane and complex as to be useful only in “black box” form, we firmly reject.

Our purpose in this book is thus to open up a large number of computational black boxes to your scrutiny. We want to teach you to take apart these black boxes and to put them back together again, modifying them to suit your specific needs. We assume that you are mathematically literate, i.e., that you have the normal mathematical preparation associated with an undergraduate degree in a physical science, or engineering, or economics, or a quantitative social science. We assume that you know how to program a computer. We do not assume that you have any prior formal knowledge of numerical analysis or numerical methods.

The scope of *Numerical Recipes* is supposed to be “everything up to, but not including, partial differential equations.” We honor this in the breach: First, we *do* have one introductory chapter on methods for partial differential equations (Chapter 19). Second, we obviously cannot include *everything* else. All the so-called “standard” topics of a numerical analysis course have been included in this book:

Sample page from NUMERICAL RECIPES IN FORTRAN 77: THE ART OF SCIENTIFIC COMPUTING (ISBN 0-521-43064-X)
Copyright (C) 1986-1992 by Cambridge University Press. Programs Copyright (C) 1986-1992 by Numerical Recipes Software.
Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one), to any server computer, is strictly prohibited. To order Numerical Recipes books or CDROMs, visit website <http://www.nr.com> or call 1-800-872-7423 (North America only), or send email to directcustserv@cambridge.org (outside North America).

linear equations (Chapter 2), interpolation and extrapolation (Chapter 3), integration (Chapter 4), nonlinear root-finding (Chapter 9), eigensystems (Chapter 11), and ordinary differential equations (Chapter 16). Most of these topics have been taken beyond their standard treatments into some advanced material which we have felt to be particularly important or useful.

Some other subjects that we cover in detail are not usually found in the standard numerical analysis texts. These include the evaluation of functions and of particular special functions of higher mathematics (Chapters 5 and 6); random numbers and Monte Carlo methods (Chapter 7); sorting (Chapter 8); optimization, including multidimensional methods (Chapter 10); Fourier transform methods, including FFT methods and other spectral methods (Chapters 12 and 13); two chapters on the statistical description and modeling of data (Chapters 14 and 15); and two-point boundary value problems, both shooting and relaxation methods (Chapter 17).

The programs in this book are included in ANSI-standard FORTRAN-77. Versions of the book in C, Pascal, and BASIC are available separately. We have more to say about the FORTRAN language, and the computational environment assumed by our routines, in §1.1 (Introduction).

Acknowledgments

Many colleagues have been generous in giving us the benefit of their numerical and computational experience, in providing us with programs, in commenting on the manuscript, or in general encouragement. We particularly wish to thank George Rybicki, Douglas Eardley, Philip Marcus, Stuart Shapiro, Paul Horowitz, Bruce Musicus, Irwin Shapiro, Stephen Wolfram, Henry Abarbanel, Larry Smarr, Richard Muller, John Bahcall, and A.G.W. Cameron.

We also wish to acknowledge two individuals whom we have never met: Forman Acton, whose 1970 textbook *Numerical Methods that Work* (New York: Harper and Row) has surely left its stylistic mark on us; and Donald Knuth, both for his series of books on *The Art of Computer Programming* (Reading, MA: Addison-Wesley), and for T_EX, the computer typesetting language which immensely aided production of this book.

Research by the authors on computational methods was supported in part by the U.S. National Science Foundation.

October, 1985

William H. Press
 Brian P. Flannery
 Saul A. Teukolsky
 William T. Vetterling